Thermophysical Properties of Gases used in Semiconductor Processing

NIST measures the thermophysical properties of process gases in response to the roadmap-expressed need of the semiconductor processing industry for gas property data. These measurements exploit novel, accurate, NIST-developed acoustic techniques. The measured properties include the speed-of-sound, ideal-gas heat capacity, density (equation of state), viscosity, and thermal conductivity.

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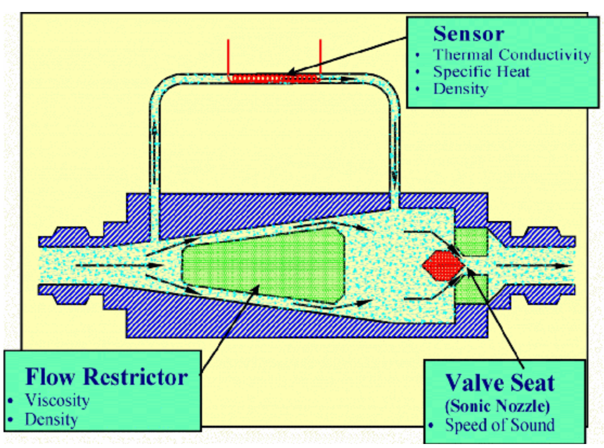
Representatives of the semiconductor industry have identified the highest priority process gases, "surrogate" gases, and the binary mixtures of process and carrier gases as well as targets for accuracy required to model manufacturing processes. Specific areas that will benefit from this work are chemical vapor deposition (CVD) processes and the calibration of mass flow controllers (MFCs) using surrogate gases. The schematic diagram below shows the components of a generic mass flow controller (MFC) and the thermophysical properties required to model them.



NIST disseminates them via the internet at the URL http://properties.nist.gov/semiprop. The database includes the heat capacity at constant pressure, thermal conductivity, viscosity, and virial coefficients $B(T)$ and $C(\mathrm{T})$ that determine the pressure-density-temperature relation of the process gas mixtures.

By the end of FY05, we used a Greenspan acoustic viscometer to measure the viscosity of 17 gases under the conditions listed in Table 1. The acoustic viscometer also determines the speed of sound in the test gas. As in the past, speed of sound was used to determine the ideal-gas heat capacity to within 0.1 % and virial coefficients that reflect each gas's non-ideality. From the virial coefficients, we developed an equation of state that predicts the gases' densities to within 0.1 %. A new resonator was employed to acquire the measurements of the last 8 gases in Table 1. Publication of these data is delayed until the theoretical model used to analyze the measurements is validated.

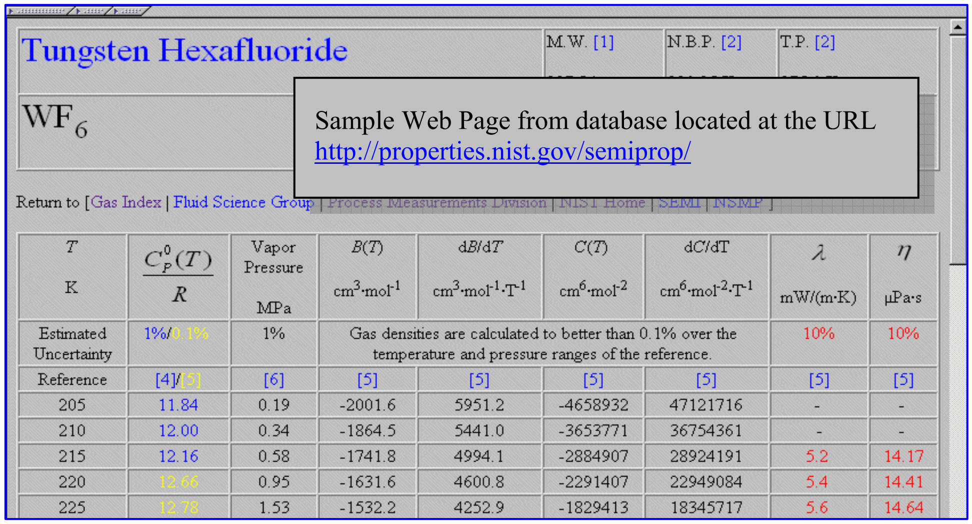
Table1. Gases and Conditions for Viscosity Data.

Gas	Temperature Range (K)	Maximum Pressure, MPa
He	298	3.3
Ar	200 - 375	3.3
N_2	298	3.3
C_3H_8	225 - 375	0.9
SF_6	298	1.8
CF_4	200 - 375	3.3
C_2F_6	225 - 375	2.8
N_2O	225 - 375	3.4
NF_3	225 - 375	3.4
BCl_3	300 - 400	1.3
Cl_2	280 - 400	3.2
HBr	225 - 400	3.3
C_4F_8	300 - 375	1.6
C0	225 - 375	2.7
$C0_2$	220 - 370	3.1
NH_3	300 - 375	3.5
SiF_4	225 - 375	2.8

The results of this research have been disseminated through publications in professional journals, by a series of talks at professional meetings, and an on-line database.

Future Plans: During FY06, we shall install a new monel spherical resonator to measure the speed of sound in the semiconductor process gases HF and SiF_4 to determine the "best in the world" equation of state for these important gases. We will complete the modeling and publish the viscosity of the hazardous process gases: Cl_2, HBr, SiF_4, C_4F_8, NH_3, CO, and CO_2. The NIST results will decrease the uncertainty of the viscosity from an estimated 10 % to approximately 0.5 %.

Dr. John Hurly is the Technical Editor of the Gases and Facilities Standards Committee of SEMI (Semiconductor Equipment and Materials International). This year, the committee gave Hurly an award for his “outstanding contributions” to the committee’s work.



Tungsten Hexafluoride

WF_6

M.W. [1]	N.B.P. [2]	T.P. [2]

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T K	$C_P^0(T)/R$	Vapor Pressure MPa	$B(T)$ $cm^3 \cdot mol^{-1}$	dB/dT $cm^3 \cdot mol^{-1} \cdot T^{-1}$	$C(T)$ $cm^6 \cdot mol^{-2}$	dC/dT $cm^6 \cdot mol^{-2} \cdot T^{-1}$	λ mW/(m·K)	η μPa·s
Estimated Uncertainty	1%/0.1%	1%	Gas densities are calculated to better than 0.1% over the temperature and pressure ranges of the reference.				10%	10%
Reference	[4]/[5]	[6]	[5]	[5]	[5]	[5]	[5]	[5]
205	11.84	0.19	-2001.6	5951.2	-4658932	47121716	-	-
210	12.00	0.34	-1864.5	5441.0	-3653771	36754361	-	-
215	12.16	0.58	-1741.8	4994.1	-2884907	28924191	5.2	14.17
220	12.66	0.95	-1631.6	4600.8	-2291407	22949084	5.4	14.41
225	12.78	1.53	-1532.2	4252.9	-1829413	18345717	5.6	14.64

Sample Web Page from database located at the URL http://properties.nist.gov/semiprop/